

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Er011-1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: Er011-1

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Bond precision:    C-C = 0.0098 A

Wavelength=0.79313

Cell:                a=9.675(5)                b=12.346(3)                c=12.523(2)  
                      alpha=80.897(16)    beta=71.847(16)    gamma=70.278(16)  
Temperature:    100 K

	Calculated	Reported
Volume	1335.7(8)	1335.7(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H5 Br4 Li O8 Zn, C4 H9 N O	?
Sum formula	C20 H14 Br4 Li N O9 Zn	C40 H28 Br8 Li2 N2 O18 Zn2
Mr	804.25	1608.54
Dx,g cm-3	2.000	2.000
Z	2	1
Mu (mm-1)	9.130	9.131
F000	772.0	772.0
F000'	766.13	
h,k,lmax	12,16,16	12,15,16
Nref	6140	5956
Tmin,Tmax	0.461,0.633	0.675,1.000
Tmin'	0.349	

Correction method= # Reported T Limits: Tmin=0.675 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.970

Theta(max)= 31.016

R(reflections)= 0.0624( 5265)

wR2(reflections)= 0.1691( 5956)

S = 1.063

Npar= 331

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

### ● Alert level C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low .	0.971	Why?
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang) .....	01D	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00982	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.715	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	144	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	11	Note
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.06A From 01D	1.01	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.91A From 032	-0.76	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H32	-0.63	eA-3

### ● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.		
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	11.26	Why ?
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.79313	Ang.
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal..(Note)	0.016	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	9	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II)	2.07	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	39	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	88	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.7	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info
PLAT984_ALERT_1_G	The Br-f' = -0.8408 Deviates from the B&C-Value	-0.8805	Check
PLAT984_ALERT_1_G	The Zn-f' = 0.2079 Deviates from the B&C-Value	0.2043	Check
PLAT985_ALERT_1_G	The Br-f" = 2.9521 Deviates from the B&C-Value	2.8944	Check
PLAT985_ALERT_1_G	The Zn-f" = 1.7386 Deviates from the B&C-Value	1.7400	Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 20 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 7 ALERT type 3 Indicator that the structure quality may be low  
 4 ALERT type 4 Improvement, methodology, query or suggestion  
 3 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

